<Bioinformatics Center> Bioknowledge Systems

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- Bioknowledge Systems -

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Scope of Research

DNA, RNA, and proteins are the basic molecular building blocks of life, but the living cell contains additional molecules, including water, ions, small chemical compounds, glycans, lipids, and other biochemical molecules, without which the cell would not function. Because the proteins responsible for biosynthesis, biodegradation, and transport of these additional molecules are encoded in the genome, one may assert that all cellular functions are specified by the genomic DNA sequence. In practice, however, it is not possible to infer higher-level systemic functions of the cell or the organism simply from the molecular sequence infomation alone. We are developing bioinformatics methods to integrate different types of data and knowledge on various aspects of the biological systems towards basic understanding of life as a molecular interaction/reaction system and also for practical applications in medical and pharmaceutical sciences.

Research Activities (Year 2008)

Grants

Kanehisa M, Knowledge Information Infrastructure for Genome Information Science, Kyoto University 21st Century COE Program, MEXT.

Kanehisa M, Backbone Database for Analysis of the Biological Systems and Environment, Grant-in-Aid for Scientific Research on Priority Areas, MEXT.

Kanehisa M, Deciphering Systemic Biological Functions by Integration of Genomic and Environmental Information, Bioinformatics Research and Development, JST.

KEGG PLANT Database

Plants produce vast and diverse natural products. These natural products are important for our lives because of their great utility as drugs and industrial materials (fibers, oils, dyes, perfumes etc.). Plants are also a major source of crude drugs. In this context, plant natural products and their biosynthetic pathways have been studied by plant scientists extensively for a long time. Recently, in the post genomic era, plant metabolomics is an important technology for plant omics research. An integrated resource of pathway and metabolite databases focused on plants is especially important for this research field.

KEGG PLANT is a new interface to the KEGG database resource, which contains an overview pathway map and sub-category pathway maps to summarize plant pathways, and hierarchical classification of plant secondary metabolites and semi-synthetic drugs from plant origin. Plant secondary metabolite pathways in KEGG PATWAY database are also extensively updated and linked to the overview and subcategory maps. Also KEGG PLANT information is linked to some KEGG DRUG compound data via hierarchical classification of semi-synthetic drugs. This useful information will help plant research and related application research field.

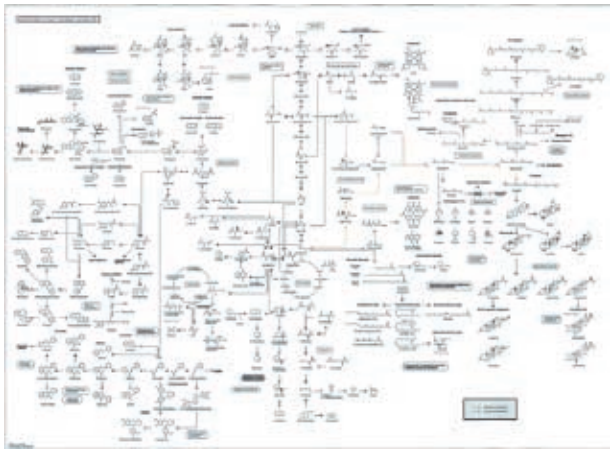

Figure 1. The KEGG PLANT Overview Map.

From the Repertoire of Desaturases and Elongases to Fatty Acid Variations

The repertoire of biosynthetic enzymes found in an organism is an important clue for elucidating the chemical structural variations of various compounds. In the case of fatty acids, it is essential to examine key enzymes that are desaturases and elongases, whose combination determine the range of fatty acid structures.

We obtained 275 desaturase and 265 elongase homologs from 56 eukaryotic genomes using PSI-BLAST. Phylogenetic and motif analysis indicated that the desaturases consist of four functionally distinct subfamilies, and the elongases consist of two subfamilies. Each subfamily has a distinct motif, whose profiles can be used for functional assignments of desaturases and elongases in newly sequenced genomes. We then predicted the ability to synthesize fatty acids, especially six types of fatty acids widely distributed in nature from the pathway view point (Figure 2). Consequently, we found that the ranges of synthesizable fatty acids are often different even between closely related organisms. The reason is that, as well as diverging into subfamilies, the enzymes have functionally diverged within the individual subfamilies. Such a variety of fatty acids may contribute to adaptation to individual environments and the ability to synthesize specific metabolites. This study provides an example of a potent strategy to bridge the gap from genomic knowledge to chemical knowledge.

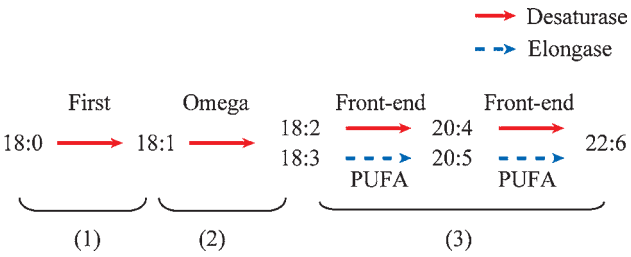

Figure 2. A schematic pathway of unsaturated fatty acids with subfamily enzymes. (1) The pathway from stearic acid (18:0) to oleic acid (18:1), catalyzed by the First subfamily. (2) The pathway from oleic acid (18:1) to linoleic acid (18:2) and alpha-linolenic acid (18:3), catalyzed by the Omega subfamily. (3) The pathway from oleic acid (18:1) and linoleic acid (18:2) to DHA (22:6), catalyzed by the Front-end subfamily the PUFA subfamily.

Kanehisa M, Integration of Genomics and Chemistry in Glycome Informatics, NIH, USA.

Goto S, Hierarchical Structuring and Integration of Knowledge in Life Sciences, Integrated Database Project, MEXT.